

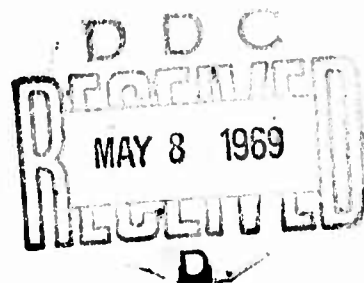
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The areas of research studied under this contract were: a) numerical methods for the integration of stiff systems of ordinary differential equations; b) computational techniques for solving sparse systems of linear equations; c) discrete methods for solving optimal control problems with state space constraints. In addition, some preliminary studies were made to see how the results of the first two areas could be most effectively employed in a design optimization package for electrical networks. At the end are a list of papers that have been published since January 1968 in outside journals, and another list of papers with the current status on their publication in a journal.



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Numerical Methods for Stiff Systems

The design of efficient numerical integration methods for stiff systems of ordinary differential equations has been studied further. The formulae designed earlier were all of a one-step type. In order to combine in those one-step methods a reasonably large order of accuracy in the conventional sense with strong, global stability and accuracy to cope with stiffness, one has to consider formulae containing higher (in particular, second) derivatives. One-step methods have the advantage of not introducing parasitic solutions, but to express the higher derivatives one must differentiate the differential equations; i. e., compute the Jacobian matrix. Recently, more attention has been focused on linear multistep methods which provide for considerable flexibility without containing higher derivatives. However, they do introduce parasitic roots. An order of accuracy $p > 2$ is not compatible with A-stability in the Dahlquist sense. Thus, slightly weaker stability concepts, which we refer to as quasi-A-stability, must be adopted in studying multistep formulae; e. g., $A(\alpha)$ -stability as defined by Widlund. A theorem has been proved which leads to a generalization of the easy-to-apply test criterion for A-stability to a general class of quasi-A-stability concepts. The analysis has been carried out in detail for circular, angular, and parabolic domains in the complex plane and applied in particular to the class of backward differentiation formulae used extensively by Gear.

It has also been possible to generalize the concept of exponential fitting, introduced earlier for one-step formulae, to multistep methods. This leads to the definition of a one-parameter family of multistep methods with global accuracy properties. As special cases, this family contains the well known closed Adams formulae (fitted at $q = 0$), and the backward differentiation formulae (fitted at infinity). It has been shown, for the class of all two-step formulae of order $p \geq 2$ whose A-stability was studied earlier, that exponential fitting is compatible with both A-stability and boundedness of the local truncation error uniformly with respect to the location of fitting.

Exponential fitting ties a given formulae to a particular problem one is solving or, more specifically, to the spectrum of the accompanying Jacobian matrix. In general, the location of fitting and the parameter in the formula then vary with the independent variable. As an alternative to exponential fitting, one can attempt to make a good a priori choice of the parameters contained in the formulae which are then kept fixed. It was shown that for the one-step, one-parameter formula $F^{(1)}$ considered in RC 1852, there exists an optimal parameter choice in a certain sense.

Sparse Matrix Theory

The computational methods for solving sparse systems of linear equations were developed further. As more applications were examined, the need for various adaptations or even new methods was recognized. Many of these were implemented, and are summarized below. In addition, it was felt that there was a diverse collection of scientists working on sparse matrices who, because they were in different scientific disciplines, did not know what had been developed in other areas. A symposium on sparse matrix methods and applications was organized and held September 9-10, 1968. The Proceedings, containing extended abstracts of the talks with complete bibliographies and the text of a panel discussion, is forthcoming, and should serve to unify the references in this field.

A major study was made of direct methods for solving linear equations as they apply to sparse matrices. The two leading methods, judged by the applications, were the various forms of Gaussian elimination and Gauss-Jordan elimination. A careful comparison was made between the elimination form of the inverse (EFI) and the product form of the inverse (PFI), respectively a form of Gaussian and Gauss-Jordan elimination. The PFI is predominantly used in the major linear programming codes in use today. One of the results of this study is that the EFI method is superior for sparse matrices in that it requires less storage and arithmetic operations than the PFI. The conclusion is that any newly developed linear programming codes should incorporate the EFI method. To give quantitative substance to this conclusion, some statistics were compiled for the computation time and storage required for both the PFI and EFI in solving systems of equations where the coefficient matrix was a sparse matrix with a random sparseness structure.

A more theoretical investigation was made to understand the fill-in phenomenon and to characterize

algorithms which require the least amount of storage. In the paper this is called s-minimal. The fill-in phenomenon refers to the fact that when one decomposes a sparse matrix into a form of its inverse, it always requires more storage; i. e., the matrix fills in. It was discovered that both the EFI and PFI as well as the Householder algorithm for factoring A into QU are not s-minimal. This means that certain computations and storage locations apparently necessary for these algorithms are really unnecessary and, therefore, waste storage and computation time. However, it was shown that if the original matrix had nonzero diagonal elements, both the EFI and the PFI are s-minimal. This result may have implications for rearrangement algorithms and explains the occurrence of almost zero elements in the linear programming codes.

Another area in sparse matrix theory that was studied was the different methods of modifying the form of the inverse when the original matrix A is changed. Five methods, some of them new, were discussed and compared. One of the methods, Kron's method, which has been discussed extensively in electrical engineering literature, was related to the method used in linear programming codes with the PFI. This analysis puts Kron's method in a new light and it seems fair to say that with sparse matrix codes available, Kron's method has little to offer.

The status of the various sparse matrix codes is summarized below.

Interpreter. This program is a modification of GNSO (an algorithm which produced FORTRAN statements for solving a given sparse system of equations). Instead of producing FORTRAN, it produces a sequence of integers which can be interpreted rapidly to produce the correct solution of a given sparse system of equations. For a problem of size 199×199 which was suggested previously by Air Force personnel, 68,250 integers were generated in 15 seconds on a 360/67. This sequence of integers

was made resident on a 2311 disk pack and had to be brought into core to solve the problem, making the execution I/O bound. Even so, it took only 3 seconds to bring in this code and solve the 199×199 system. The CPU was idle $1/6$ of the time.

Compiler. A special purpose compiler was designed and implemented to work with GNSO. This compiler translates code generated by GNSO into IBM 360 machine executable code. The need for such a compiler was that either the standard FORTRAN compiler was too slow, or could not compile the size of program generated by GNSO. For example, on a problem of size 57×57 , FORTRAN H failed to compile the FORTRAN statements produced by GNSO because there were too many statements, FORTRAN G took 9 minutes, and the new special compiler took 1 second. GNSO and the compiler took 29 seconds to produce the code for the 199×199 problem. This code executes in .2 seconds.

New GNSO. A new version of GNSO based on a monotone sequence of integers representing the nonzero entries of a sparse matrix was implemented. This replaces the use of the bit map in GNSO and is more efficient for large matrices.

Band Matrix Program. This is a special program for sparse matrices which have a band structure; i. e., all the nonzero elements lie in a band about the diagonal. The program is coded in FORTRAN, but in the parts of the code which are the most repetitive, machine language is used to achieve maximum efficiency. For computers like the IBM 360 models 91 and 95, the program takes full advantage of the loop mode so that maximum utilization of the CPU can be approached.

Sparse Matrix Gaussian Elimination. Three programs based on Gaussian elimination have been developed. These codes are aimed at applications where the problem is solved only once and not repeatedly with the same

sparseness structure. One code uses column ordering, one uses row ordering, while the third combines row-column permutations to achieve reduced fill-in and increased accuracy. Also, a sparse matrix program for Gauss-Jordan elimination was coded to be used for comparison purposes. .

Solution of Optimal Control Problems

Work was continued on the problem of the computation of solutions of continuous optimal control problems, with the goal of obtaining a procedure for solving problems with intermediate state constraints. In an earlier report, it was proved that problems with convex costs, linear differential systems, and any type of control and trajectory constraints can be approximated by discrete (finite-dimensional) optimal control problems. The proof given was semiconstructive. These theoretical results were tested on several minimum energy, fuel, and time problems with intermediate control constraints and terminal state constraints. The discrete approximations, obtained by directly discretizing these problems, were solved by linear and quadratic programming algorithms. The computed optimal costs, controls, and trajectories were compared with the solutions obtained analytically. The results demonstrated that discretization is a feasible method for these types of problems.

One minimum time problem with intermediate state constraints was also solved by this technique, but the computation was extremely inefficient and resulted in excessively large computational times. Effort is presently being exerted to utilize the sparseness of the matrices in the problems generated to obtain reasonable computing times.

Time was spent studying existing methods for tackling problems with intermediate state constraints. There are essentially two approaches: (1) utilizing the associated necessary conditions for optimality; and (2) introducing penalty functions. Approach (1) requires a priori knowledge of the optimal trajectory and is very difficult even for linear systems. Approach (2) is a direct method, but requires delicate treatment numerically. It was proved theoretically that approach (2), if used to remove all state constraints, yields the solution to the problem to be solved if and only if the problem is the same as its relaxation. By example, it was also demonstrated that if (2) is used to remove only the intermediate

state constraints, the results obtained may be the solution of the original problem or the solution of its relaxation. Hence, if this technique is applied to a problem that is not the same as its relaxation, care should be exercised. (Observe that if the problem is linear with a convex cost, then it is the same as its relaxation.) It is conjectured that this result will be true for approach (3) (direct discretization), too.

Optimal Design of Electrical Networks

It has been recognized for some time that the problem of finding the optimal parameter values for a given network and a given performance criterion involves the numerical calculation of the transient response of the network equations and the adjoint equations. With this information, one can compute the gradient direction of the performance criterion with respect to the parameters. The parameters are then changed in an appropriate way and this procedure is then repeated. The optimum design is then obtained after many iterations, each one requiring perhaps 1000 to 10,000 time-step calculations. If the basic time-step computation is not efficient, the computation time required can be unacceptable. Since one is involved with stiff systems in electrical networks as well as nonlinear devices in many practical design problems, the basic time-step calculation requires the solution of a system of linear equations, perhaps several times.

A preliminary study of this problem, starting with the topological description of the network, has led to the conclusion that network analysis can be viewed basically as Gaussian elimination for a large, very sparse, matrix. This point of view gives a uniform approach to network analysis which allows one to write a simple network analysis package. The main computation is based on several of the sparse matrix codes already developed. In addition, because of its simplicity, the method allows the inclusion of the most general electrical elements (e. g., voltage controlled voltage sources) and is easily adapted to optimal design problems. It also frees one of some inhibiting ideas, about how networks should be solved, that have developed in recent years. Since many of these ideas were developed without a knowledge of sparse matrices, they may be inefficient compared to the newer techniques.

The conclusions of this study are that a new network analysis and optimal design package should be

developed, and this is currently underway. In addition, by modifying some of the sparse matrix codes, to take advantage of the special nature of the network problems, even better efficiencies can be achieved.

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